

# Two-species Bose-Einstein condensate in an optical lattice: analytical approximate formulæ.

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Employing a general variational method and perturbation theory, we derived explicit solutions for the description of one-dimensional two species Bose-Einstein condensates confined by a harmonic trap potential in an optical lattice. We consider the system of two coupled Gross-Pitaevskii equations (GPE) and derive explicit expressions for the chemical potentials and wavefunctions in terms of the atom-atom interaction parameters and laser intensity. We have compared our results with the numerical solutions of the GPE and performed a quantitative analysis for the both considered methods. We underline the importance of the obtained explicit solutions to characterize the density profile or degree of miscibility of the two components.

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## I. INTRODUCTION

Multiple Bose-Einstein condensates (BEC) of different atomic species have been realized in the last years. Mixture of alkali atoms of  $^{87}\text{Rb}$  in two different hyperfine internal spin states,<sup>1</sup> atoms  $^{23}\text{Na}$  with a superposition of spinor condensates,<sup>2</sup> combination of  $^{41}\text{K}$  -  $^{87}\text{Rb}$ ,<sup>3</sup>  $^{87}\text{Rb}$ - $^{85}\text{Rb}$ ,<sup>4</sup>  $^{87}\text{Rb}$ - $^{133}\text{Cs}$ ,<sup>5</sup> and gases of rare atomic species  $^{168}\text{Yb}$ - $^{174}\text{Yb}$ ,<sup>6</sup> have been employed to produce two species BEC. These quantum degenerate mixtures allow to study several intriguing phenomena as the dynamics of the superfluid system,<sup>2,3</sup> the production of heteronuclear polar molecules,<sup>7</sup> the miscibility or immiscibility of the two quantum fluids,<sup>8</sup> among other effects. Also, two-species BEC loaded in an optical lattice have been explored.<sup>9,10</sup> A similar system but of Fermi-Bose quantum gas mixture in a 3-dimensional optical lattice was implemented to study the interfering paths of the bosonic wave function scattered by the presence of fermionic atoms.<sup>11</sup> These results have led to an intense theoretical and mathematical studies on the properties of the two-coupled Gross-Pitaevskii equations.

The basis of this research lies on the knowledge of the dependence of the chemical potentials as functions of the interparticle interactions and the spatial density probability.<sup>12</sup>

A fascinating experimental realization to study the one dimensional (1D) transport properties of ultracold fermionic and bosonic atoms in a periodic potential have been reported in Ref.12.

From the theoretical point of view there are several studies for the description of two species Bose conden-

sates. Typically, numerical approaches or Thomas-Fermi approximation are employed to calculate the chemical potential and the ground state wave functions.<sup>13</sup> In Ref.14 it is analyzed the mixture of 1D two interacting condensates modeled by the Bose-Hubbard Hamiltonian and by using the quantum Monte Carlo numerical simulations. Theoretical analysis of the 1D two component BEC problem becomes an important reservoir to mimic different physical effects of the Condensed Matter Physics (see for example Refs.15–17), including the magnetic properties of the bosonic mixtures with tunable interspecies interactions.<sup>18</sup> Also, as it will be shown below, we can take advantage of analytical results for the study of quantum effects and predictions for cold atoms researches.

Assuming a “cigar-shaped” type for the Bose-Einstein condensates<sup>19,20</sup> of a gas composed by two kind of bosons loaded in an optical lattice, we can consider the following system of 1D GP equations:

$$\mathbf{L}_0 \Phi + [\mathbf{L}_I - \nu] \Phi = \mathbf{0}, \quad (1)$$

where  $\mathbf{L}_0$  and  $\mathbf{L}_I$  are, respectively the operators

$$\begin{bmatrix} -\frac{\hbar^2}{2m_1} \frac{d^2}{dx^2} + \frac{1}{2} m_1 \omega_1^2 x^2 & 0 \\ 0 & -\frac{\hbar^2}{2m_2} \frac{d^2}{dx^2} + \frac{1}{2} m_2 \omega_2^2 x^2 \end{bmatrix}, \quad (2)$$

$$\begin{bmatrix} \overline{\lambda_1} |\Phi_1|^2 - V_L \cos^2\left(\frac{2\pi x}{d}\right) & \overline{\lambda_3} \Phi_1 \Phi_2 \\ \overline{\lambda_3} \Phi_1 \Phi_2 & \overline{\lambda_2} |\Phi_2|^2 - V_L \cos^2\left(\frac{2\pi x}{d}\right) \end{bmatrix}, \quad (3)$$

and

$$\Phi = \begin{bmatrix} \Phi_1 \\ \Phi_2 \end{bmatrix}, \quad \nu = \begin{bmatrix} \nu_1 \\ \nu_2 \end{bmatrix}. \quad (4)$$

Here,  $\omega_i > 0$  denotes the harmonic trap frequencies where for simplicity we consider the same for both condensates, i.e.,  $\omega_1 = \omega_2 = \omega$ ,  $m_i > 0$ , and  $\nu_i$  are, respectively, the mass and chemical potential for the specie  $i$  ( $i = 1$  and  $2$ ),  $V_L > 0$  and  $d > 0$  the intensity and laser wavelength,  $\bar{\lambda}_i$  takes into account the self-interaction term for the  $i$ th specie, and  $\lambda_3$ , the interaction between unlike particles of the species 1 and 2. In this system, the complex function  $\Phi_i(x)$  is known<sup>19</sup> as the *macroscopic wavefunction* or *order parameter* of the  $i$ th component and is defined as the expectation value of the corresponding field operator, namely  $\Phi_i(x) = \langle \hat{\Phi}_i(x) \rangle$ . The functions  $\Phi_i$  satisfy the normalization conditions

$$\int_{\mathbb{R}} |\Phi_i(x)|^2 dx = N_i, \quad i = 1, 2, \quad (5)$$

where  $N_i$  denotes the number of atoms of the  $i$ th specie.

It is worth to notice that in some situations, as in the case of *spinor condensates*, where one produces confinement of an atomic cloud of an element in different spin states,<sup>19,21</sup> the condition (5) must be substituted by

$$\int_{\mathbb{R}} |\Phi_1(x)|^2 dx + \int_{\mathbb{R}} |\Phi_2(x)|^2 dx = N, \quad N = N_1 + N_2.$$

We can rewrite the system (1) in its dimensionless form, by considering, for instance,  $l = \sqrt{\hbar/(m_1\omega)}$ ,  $x = l\xi$ , and  $\Phi_i(x) = \psi_i(\xi)/\sqrt{l}$ ,  $i = 1, 2$ , in which case we have

$$\mathcal{L}_0 \Psi + [\mathcal{L}_I - \mu] \Psi = 0, \quad (6)$$

where  $\mathcal{L}_0$  and  $\mathcal{L}_I$  are respectively the operators

$$\begin{bmatrix} -\frac{1}{2} \frac{d^2}{d\xi^2} + \frac{1}{2} \xi^2 & 0 \\ 0 & -\frac{a_2}{2} \frac{d^2}{d\xi^2} + \frac{1}{2a_2} \xi^2 \end{bmatrix}, \quad (7)$$

$$\begin{bmatrix} \lambda_1 |\psi_1|^2 - V_0 \cos^2(\alpha\xi) & \lambda_3 \psi_1 \psi_2 \\ \lambda_3 \psi_1 \psi_2 & \lambda_2 |\psi_2|^2 - V_0 \cos^2(\alpha\xi) \end{bmatrix}, \quad (8)$$

$$\Psi = \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}, \quad \mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}. \quad (9)$$

Here,  $a_2 = m_1/m_2$ ,  $\lambda_i = \bar{\lambda}_i/l\hbar\omega$ , ( $i = 1, 2, 3$ ),  $V_0 = V_L/\hbar\omega$ ,  $\alpha = 2l\pi/d$  and  $\mu_j = \nu_j/\hbar\omega$  ( $j = 1, 2$ ). For the system (6), the energy functional can be cast as

$$\begin{aligned} \mathbf{E}(\psi_1, \psi_2) &= E_1(\psi_1) + E_2(\psi_2) \\ &+ \frac{\lambda_3}{2} \int_{\mathbb{R}} |\psi_1(\xi)|^2 |\psi_2(\xi)|^2 d\xi, \end{aligned} \quad (10)$$

with

$$\begin{aligned} E_1(\psi) &= \frac{1}{4} \int_{\mathbb{R}} |\psi'(\xi)|^2 d\xi + \frac{1}{4} \int_{\mathbb{R}} \xi^2 |\psi(\xi)|^2 d\xi + \\ &\frac{\lambda_1}{4} \int_{\mathbb{R}} |\psi(\xi)|^4 d\xi - \frac{V_0}{2} \int_{\mathbb{R}} \cos^2(\alpha\xi) |\psi(\xi)|^2 d\xi, \\ E_2(\psi) &= \frac{a_2}{4} \int_{\mathbb{R}} |\psi'(\xi)|^2 d\xi + \frac{1}{4a_2} \int_{\mathbb{R}} \xi^2 |\psi(\xi)|^2 d\xi + \\ &\frac{\lambda_2}{4} \int_{\mathbb{R}} |\psi(\xi)|^4 d\xi - \frac{V_0}{2} \int_{\mathbb{R}} \cos^2(\alpha\xi) |\psi(\xi)|^2 d\xi. \end{aligned}$$

Therefore, the partial Fréchet derivatives of  $\mathbf{E}$  are

$$\partial_1 \mathbf{E} = E'_1(\psi_1) + \lambda_3 |\psi_2(\xi)|^2 \psi_1(\xi), \quad (11)$$

$$\partial_2 \mathbf{E} = E'_2(\psi_2) + \lambda_3 |\psi_1(\xi)|^2 \psi_2(\xi). \quad (12)$$

The minimum of the energy  $\mathbf{E}(\psi_1, \psi_2)$  under the restrictions  $\int_{\mathbb{R}} |\psi_i(\xi)|^2 d\xi = N_i$  satisfies the Lagrange conditions for some constants  $\mu_i/2$  ( $i = 1, 2$ ),

$$\partial_1 \mathbf{E} = \mu_1 \psi_1(\xi), \quad \partial_2 \mathbf{E} = \mu_2 \psi_2(\xi). \quad (13)$$

Notice that (13) coincides with (6).

In previous works,<sup>22–25</sup> we have presented different methods to express the chemical potential  $\mu$  and the order parameter  $\psi(\xi)$  as function of the interaction parameter  $\lambda$  for the 1D Gross-Pitaevskii equation. In the present paper, we adapt two of these methods (the generalized variational approach<sup>25</sup> and perturbation theory) for the system (6), by considering the vector chemical potential  $\mu$  as function of the atom-atom interaction strength of each component  $\lambda_1$ ,  $\lambda_2$  and the interaction between both species,  $\lambda_3$ .

The paper is organized as follows: in Section II we present the mathematical framework of the variational problem formulation, which characterizes the condensate as ground state solution for the system (6), as well as its equivalent integral representation. We also report an exact representation of  $\mu(\lambda_1, \lambda_2, \lambda_3)$  over which is based our variational approach described in Section III. In Section IV we develop the perturbation method valid for two coupled GP equations. Section V is devoted to present the results of these two approaches comparing with the exact numerical solution of the system (6). Also, final conclusions are delivered showing the range of validity of both considered methods, with respect to parameter values employed for the description of two-species Bose-Einstein condensate in an optical lattice.

## II. GENERAL MATHEMATICAL FRAMEWORK

In this section we establish the functional framework for the mathematical analysis of existence, regularity and stability of ground state solutions for the system (6). There is a great number of mathematical work on these questions, some of them mentioned in the references below. The eigenvalue problem (6) has an intrinsic mathematical interest, but the ground state solutions (i.e.,

standing wave solutions of minimal energy) play important role for condensates. By standing wave we mean solution of the evolution equation

$$i \frac{\partial \Psi}{\partial t} = [\mathcal{L}_0 + \mathcal{L}_I] \Psi, \quad (14)$$

of the form

$$\Psi(t, \xi) = \begin{bmatrix} \exp(-i\mu_1 t) \psi_1(\xi) \\ \exp(-i\mu_2 t) \psi_2(\xi) \end{bmatrix}.$$

### A. Existence of ground states and their stability

We consider the following minimization problem

$$\mathbf{E}_{min}(\lambda) = \min\{\mathbf{E}(\Psi); \Psi \in \Sigma\}, \quad (15)$$

where  $\lambda = (\lambda_1, \lambda_2, \lambda_3)$ ,  $\Psi = (\psi_1, \psi_2)$ ,

$$\Sigma = \left\{ \Psi \in \Xi; \int_{\mathbb{R}} |\psi_1(\xi)|^2 d\xi = N_1, \int_{\mathbb{R}} |\psi_2(\xi)|^2 d\xi = N_2 \right\}$$

and  $\Xi = \mathcal{V} \times \mathcal{V}$ , where

$$\mathcal{V} = \left\{ \psi \in H^1(\mathbb{R}); \int_{\mathbb{R}} [|\psi'(\xi)|^2 + \xi^2 |\psi(\xi)|^2] d\xi < \infty \right\}$$

and  $H^1(\mathbb{R})$  is the standard Sobolev space.

Although the solutions of Eq. (6) are in general complex valued functions, we can restrict ourselves to just the real valued ones. This can easily be justified because any solution of this system satisfies the following inequality:<sup>26</sup> there exist  $0 < \delta \leq 1$  and  $C(\delta) > 0$  such that

$$|\Psi(\xi)|^2 + |\Psi'(\xi)|^2 \leq C(\delta) \exp(-\delta \xi^2), \quad \forall \xi \in \mathbb{R}. \quad (16)$$

Indeed, assuming that

$$\Psi(\xi) = \begin{bmatrix} \psi_{1R}(\xi) + i\psi_{1I}(\xi) \\ \psi_{2R}(\xi) + i\psi_{2I}(\xi) \end{bmatrix}, \quad (17)$$

the exponential decay (16) and a simple calculus gives

$$\psi'_{1R} \psi_{1I} - \psi_{1R} \psi'_{1I} = \frac{d}{d\xi} \left( \frac{\psi_{1R}}{\psi_{1I}} \right) |\psi_{1I}|^2 = 0.$$

Therefore,  $\psi_{1R} = \beta \psi_{1I}$  for some real constant  $\beta \neq 0$ . The same holds for second component of  $\Psi$ , which gives us  $\psi_{2R} = \gamma \psi_{2I}$  for some constant  $\gamma$ . Hence, the function

$$\mathbf{U}(\xi) = \begin{bmatrix} \sqrt{1 + \beta^2} \psi_{1R}(\xi) \\ \sqrt{1 + \gamma^2} \psi_{2R}(\xi) \end{bmatrix} \quad (18)$$

is a real solution of (6) and (17) is given by

$$\Psi(\xi) = \begin{bmatrix} \left( \frac{1}{\sqrt{1 + \beta^2}} + \frac{i\beta}{\sqrt{1 + \beta^2}} \right) \psi_{1R}(\xi) \\ \left( \frac{1}{\sqrt{1 + \gamma^2}} + \frac{i\gamma}{\sqrt{1 + \gamma^2}} \right) \psi_{2R}(\xi) \end{bmatrix} \quad (19)$$

The existence of a minimal energy solution is a consequence of the Gagliardo-Nirenberg inequality (see Theorem 1.3.7 in Ref.27), which in 1D allows us to show that the energy functional  $\mathbf{E}$  is bounded by below on the manifold  $\Sigma$ , for all values of  $\lambda_i \in \mathbb{R}$ ,  $i = 1, 2, 3$ . With arguments of convexity, we can show that the (real) solution of minimal energy is unique provided that  $\lambda_1, \lambda_2$  and  $\lambda_3$  are positive. Moreover, since the system (6) has the properties of conservation of energy and mass (i.e., the number of particles), we can prove the *orbital stability*<sup>25,28</sup> of ground states.

On the other hand, the space  $\mathcal{H} = L^2(\mathbb{R}) \times L^2(\mathbb{R})$  is a Hilbert space if one considers the usual inner product

$$(\Psi | \Phi)_{\mathcal{H}} = \int_{\mathbb{R}} \psi_1(\xi) \phi_1(\xi) d\xi + \int_{\mathbb{R}} \psi_2(\xi) \phi_2(\xi) d\xi$$

and the differential operator

$$\mathcal{L}_0 : D(\mathcal{L}_0) \subset \mathcal{H} \rightarrow \mathcal{H}$$

is self-adjoint and maximal monotone.<sup>29</sup> So, it is invertible and we can rewrite the equation (6) as

$$\Psi = \mathcal{L}_0^{-1} [\mu - \mathcal{L}_I] \Psi. \quad (20)$$

Since  $D(\mathcal{L}_0) \subset \Xi$  and  $\Xi$  is compactly embedded in  $\mathcal{H}$ ,<sup>25</sup>  $\mathcal{L}_0^{-1}$  is a compact integral operator.

### B. Exact formulæ

We assume that, for each  $\lambda \in \mathbb{R}^3$ , we can choose  $\Psi_\lambda \in \Sigma$  such that the map  $\lambda \mapsto \Psi_\lambda$  is a differentiable manifold in  $\Xi$ . Then, we have

$$\begin{aligned} \frac{\partial \mathbf{E}_{min}}{\partial \lambda_1}(\lambda) &= \left\langle E'_1(\psi_{1\lambda}) : \frac{\partial}{\partial \lambda_1} \psi_{1\lambda} \right\rangle + \frac{1}{4} \|\psi_{1\lambda}\|_4^4 \\ &\quad + \left\langle E'_2(\psi_{2\lambda}) : \frac{\partial}{\partial \lambda_1} \psi_{2\lambda} \right\rangle \\ &\quad + \lambda_3 \left\langle |\psi_{2\lambda}|^2 \psi_{1\lambda} : \frac{\partial}{\partial \lambda_1} \psi_{1\lambda} \right\rangle \\ &\quad + \lambda_3 \left\langle |\psi_{1\lambda}|^2 \psi_{2\lambda} : \frac{\partial}{\partial \lambda_1} \psi_{2\lambda} \right\rangle \\ &= \mu_1(\lambda) \frac{\partial}{\partial \lambda_1} \|\psi_{1\lambda}\|_2^2 + \mu_2(\lambda) \frac{\partial}{\partial \lambda_1} \|\psi_{2\lambda}\|_2^2 \\ &\quad + \frac{1}{4} \|\psi_{1\lambda}\|_4^4. \end{aligned}$$

Since  $(\psi_{1\lambda}, \psi_{2\lambda}) \in \Sigma$  implies

$$\frac{\partial}{\partial \lambda_1} \|\psi_{1\lambda}\|_2^2 = \frac{\partial}{\partial \lambda_1} \|\psi_{2\lambda}\|_2^2 = 0,$$

we get

$$\frac{\partial \mathbf{E}_{min}}{\partial \lambda_1}(\lambda) = \frac{1}{4} \|\psi_{1\lambda}\|_4^4.$$

*Mutatis-mutandis*, we have

$$\frac{\partial \mathbf{E}_{min}}{\partial \lambda_2}(\lambda) = \frac{1}{4} \|\psi_{2\lambda}\|_4^4$$

and with the same arguments, we obtain

$$\frac{\partial \mathbf{E}_{min}}{\partial \lambda_3}(\lambda) = \frac{1}{2} \|\psi_{1\lambda} \psi_{2\lambda}\|_2^2.$$

Therefore,

$$\nabla \mathbf{E}_{min}(\lambda) = \left( \frac{1}{4} \|\psi_{1\lambda}\|_4^4, \frac{1}{4} \|\psi_{2\lambda}\|_4^4, \frac{1}{2} \|\psi_{1\lambda} \psi_{2\lambda}\|_2^2 \right)$$

and

$$\mathbf{E}_{min}(\lambda) = \mathbf{E}_{min}(0) + \int_0^1 \nabla \mathbf{E}_{min}(\lambda(s)) \cdot \frac{d}{ds} \lambda(s) ds,$$

for any smooth path  $\lambda(s)$  in  $\mathbb{R}^3$  joining the points  $(0, 0, 0)$  and  $(\lambda_1, \lambda_2, \lambda_3)$ . In particular, for the linear path  $\lambda(s) = s\lambda = (s\lambda_1, s\lambda_2, s\lambda_3)$ ,  $0 \leq s \leq 1$ , for which we have the following formula

$$\begin{aligned} \mathbf{E}_{min}(\lambda) &= \mathbf{E}_{min}(0, 0, 0) + \frac{1}{4} \int_0^1 \left( \|\psi_{s1\lambda}\|_4^4 \lambda_1 \right. \\ &\quad \left. + \|\psi_{s2\lambda}\|_4^4 \lambda_2 + 2\|\psi_{s1\lambda} \psi_{s2\lambda}\|_2^2 \lambda_3 \right) ds. \end{aligned} \quad (21)$$

The chemical potentials  $\mu_1$  and  $\mu_2$  as function of the parameter  $\lambda$  can be easily calculated by multiplying the first equation of (6) by  $\psi_{1\lambda}$ , the second by  $\psi_{2\lambda}$  and taking the integral over  $\mathbb{R}$ . By this calculation, we get

$$\mu_1(\lambda) = \frac{2}{N_1} \left( E_1(\psi_{1\lambda}) + \frac{\lambda_1}{4} \|\psi_{1\lambda}\|_4^4 + \frac{\lambda_3}{2} \|\psi_{1\lambda} \psi_{2\lambda}\|_2^2 \right), \quad (22)$$

$$\mu_2(\lambda) = \frac{2}{N_2} \left( E_2(\psi_{2\lambda}) + \frac{\lambda_2}{4} \|\psi_{2\lambda}\|_4^4 + \frac{\lambda_3}{2} \|\psi_{1\lambda} \psi_{2\lambda}\|_2^2 \right). \quad (23)$$

### III. VARIATIONAL APPROACH

We consider the following trial functions:

$$\psi_k(\xi) = \sqrt{N_k} \left( \frac{2\tau_k}{\pi} \right)^{1/4} \exp(-\tau_k \xi^2), \quad k = 1, 2. \quad (24)$$

By calculating the energy  $\mathbf{E}$  with these functions, we get:

$$\begin{aligned} \mathbf{E}(\psi_1, \psi_2) &= \sum_{k=1}^2 N_k \left( \frac{a_k}{4} \tau_k + \frac{1}{16a_k \tau_k} + \frac{\lambda_k N_k \tau_k^{1/2}}{4\sqrt{\pi}} \right. \\ &\quad \left. - \frac{V_0}{4} \left( 1 + e^{-\alpha^2/2\tau_k} \right) \right) \\ &\quad + \frac{\lambda_3 N_1 N_2}{\sqrt{2\pi}} \left( \frac{\tau_1 \tau_2}{\tau_1 + \tau_2} \right)^{1/2}. \end{aligned}$$

where, to simplify the notation, we introduced  $a_1 = 1$ . So, by denoting  $f(\tau_1, \tau_2) = \mathbf{E}(\psi_1, \psi_2)$ , it is easy to see that  $f(\tau_1, \tau_2)$  is bounded by bellow. Indeed, if  $\lambda_3 \geq 0$ , we have

$$\begin{aligned} f(\tau_1, \tau_2) &\geq \sum_{k=1}^2 N_k \left( \frac{a_k}{4} \tau_k + \frac{1}{16a_k \tau_k} + \frac{\lambda_k N_k}{4\sqrt{\pi}} \tau_k^{1/2} \right. \\ &\quad \left. - \frac{V_0}{4} \left( 1 + e^{-\alpha^2/2\tau_k} \right) \right) \end{aligned}$$

and the conclusion is evident. Otherwise, notice that

$$\begin{aligned} \left( \frac{\tau_1 \tau_2}{\tau_1 + \tau_2} \right)^{1/2} &\leq \frac{1}{2} \sqrt{\tau_1 + \tau_2} \leq \frac{\sqrt{2}}{2} \max\{\sqrt{\tau_1}, \sqrt{\tau_2}\} \\ &\leq \frac{\sqrt{2}}{2} (\sqrt{\tau_1} + \sqrt{\tau_2}), \quad \forall \tau_1, \tau_2 > 0 \end{aligned}$$

from which we get

$$\begin{aligned} f(\tau_1, \tau_2) &\geq \sum_{k=1}^2 N_k \left[ \frac{a_k}{4} \tau_k + \frac{1}{16a_k \tau_k} \right. \\ &\quad \left. + \frac{1}{2\sqrt{\pi}} \left( \frac{\lambda_k N_k}{2} + \frac{\lambda_3 N_1 N_2}{N_k} \right) \sqrt{\tau_k} \right. \\ &\quad \left. - \frac{V_0}{4} \left( 1 + e^{-\alpha^2/2\tau_k} \right) \right]. \end{aligned}$$

Hence,  $f(\tau_1, \tau_2)$  reaches its minimum at some  $\tau_k(\lambda_1, \lambda_2, \lambda_3)$ , ( $k = 1, 2$ ) which are necessarily solutions of the algebraic system ( $i \neq j$ ):

$$\begin{aligned} a_i^2 \tau_i^2 + \frac{\lambda_i N_i a_i}{2\sqrt{\pi}} \tau_i^{3/2} + \frac{2\lambda_3 N_1 N_2 a_i}{\sqrt{2\pi} N_i} \left( \frac{\tau_i \tau_j}{\tau_i + \tau_j} \right)^{3/2} \\ - \frac{V_0 \alpha^2 a_i}{2} e^{-\alpha^2/2\tau_i} = \frac{1}{4}, \quad i \neq j. \end{aligned} \quad (25)$$

These are the equations to be solved in order to obtain  $\tau_1(\lambda)$  and  $\tau_2(\lambda)$  which will be used in the formulas of  $\mu_{app,1}(\lambda)$  and  $\mu_{app,2}(\lambda)$  (see below). Notice that if  $\lambda_1 \neq \lambda_2$ , the respective roots are different even in the case  $V_0 = 0$ ,  $N_1 = N_2 = N$  and  $m_1 = m_2$ . Indeed, by subtracting the first equation from the second one in (25), we obtain:

$$\tau_2^2 - \tau_1^2 = \frac{N}{2\sqrt{\pi}} [\lambda_1 \tau_1^{3/2} - \lambda_2 \tau_2^{3/2}],$$

and we see that, if  $\tau_1 = \tau_2$ , then  $\lambda_1 \tau_1^{3/2} - \lambda_2 \tau_2^{3/2} = 0$ , which implies that  $\lambda_1 = \lambda_2$ .

By choosing,  $\sigma_i = \sqrt{a_i \tau_i}$ ,  $i = 1, 2$ , the equations (25) can be written as

$$\begin{aligned} \sigma_i^4 + \frac{\Lambda_i}{2\sqrt{\pi}} \sigma_i^3 + \frac{\sqrt{2} \Lambda_{ij} a_i \sqrt{a_j}}{\sqrt{\pi}} \left( \frac{\sigma_i^2 \sigma_j^2}{a_j \sigma_i^2 + a_i \sigma_j^2} \right)^{3/2} \\ - \frac{V_0 \alpha^2 a_i}{2} e^{-\alpha^2 a_i / 2 \sigma_i^2} = \frac{1}{4}, \quad i \neq j, \end{aligned} \quad (26)$$

where, for  $i \neq j$ ,  $\Lambda_i = \lambda_i N_i / \sqrt{a_i}$  and  $\Lambda_{ij} = \lambda_3 N_j / \sqrt{a_j}$ .

### A. Approximate formulæ

Let  $\sigma_1(\Lambda)$  and  $\sigma_2(\Lambda)$  with  $\Lambda = (\Lambda_1, \Lambda_2, \Lambda_{12}, \Lambda_{21})$ , the solution of the system (26).

Using Eqs. (22) and (23), a direct calculation gives:

$$\begin{aligned} \mu_{app,1}(\Lambda) = & \frac{\sigma_1^2(\Lambda)}{2} + \frac{1}{8\sigma_1^2(\Lambda)} + \frac{\Lambda_1}{\sqrt{\pi}}\sigma_1(\Lambda) \\ & - \frac{V_0}{2} \left(1 + e^{-\alpha^2/2\sigma_1^2(\Lambda)}\right) \\ & + \frac{\sqrt{2}\Lambda_{12}\sqrt{a_2}}{\sqrt{\pi}} \left(\frac{\sigma_1^2(\Lambda)\sigma_2^2(\Lambda)}{a_2\sigma_1^2(\Lambda) + \sigma_2^2(\Lambda)}\right)^{1/2}, \end{aligned} \quad (27)$$

$$\begin{aligned} \mu_{app,2}(\Lambda) = & \frac{\sigma_2^2(\Lambda)}{2} + \frac{1}{8\sigma_2^2(\Lambda)} + \frac{\Lambda_2}{\sqrt{\pi}}\sigma_2(\Lambda) \\ & - \frac{V_0}{2} \left(1 + e^{-\alpha^2 a_2/2\sigma_2^2(\Lambda)}\right) \\ & + \frac{\sqrt{2}\Lambda_{21}}{\sqrt{\pi}} \left(\frac{\sigma_1^2(\Lambda)\sigma_2^2(\Lambda)}{a_2\sigma_1^2(\Lambda) + \sigma_2^2(\Lambda)}\right)^{1/2}. \end{aligned} \quad (28)$$

### B. Properties of the wavefunction and the minimal energy

As it was pointed out in Eq. (16), each component of  $\Psi(\xi)$  in Eq. (9) behaves as a Gaussian as  $\xi \rightarrow \pm\infty$ , for all values of  $\Lambda$ ,  $\mu$  and  $V_0$ . In a general way, this behaviour justify the selection of the trial function (24). Nevertheless, as it is achieved in Fig. (1), the variation of the wavefunction of one specie with respect to the optical lattice intensity,  $V_0 = V_L/\hbar\omega$  and the reduced wavelength,  $\alpha^{-1} = d/(2l\pi)$  cannot be accounted by a Gaussian trial function (24). The strong variation of the optical lattice potential  $U(\xi) = -V_0 \cos^2(\alpha\xi)$  with respect to  $\alpha$  and  $V_0$ , keep off the contribution of the monotonic behavior of the harmonic potential  $\xi^2$  to order parameter. Thus, the variational approach presented here does not allow good results in the case  $V_0 \neq 0$  is large enough. Indeed, by an effective numerical solution of the 1D Gross-Pitaevskii equation we obtain the order parameter  $\psi(\xi)$  as shown in Figure 1. On the other hand, if we consider the equivalent formula of (25) for the one component BEC, we obtain<sup>25</sup>

$$\sigma^4 + \frac{\lambda}{4\sqrt{\pi}}\sigma^3 - \frac{V_0\alpha^2}{4}e^{-\alpha^2/2\sigma^2} = \frac{1}{4}. \quad (29)$$

For  $\lambda \geq 0$  fixed, the function  $\sigma(V_0)$  implicitly defined by Eq. (29) satisfies the differential equation

$$\frac{d\sigma}{dV_0} = \frac{\alpha^2 e^{-\alpha^2/2\sigma^2}}{16\sigma^3 + \frac{3\lambda}{\sqrt{\pi}}\sigma^2 - \frac{V_0\alpha^4}{\sigma^3}e^{-\alpha^2/2\sigma^2}} \quad (30)$$

which shows that it is increasing and blows up for a certain  $V_0$  large enough.

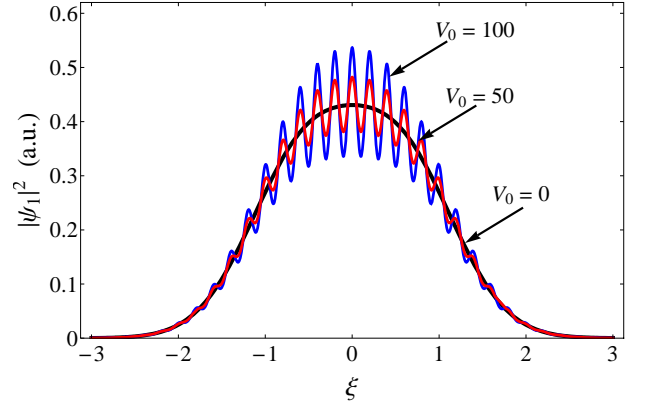


FIG. 1: (Color online) Normalized density probability for the order parameter of one specie,  $|\psi_1(\xi)|^2$  ( $\Lambda_3 = 0$ ), for  $\Lambda_1 = 2$ ,  $d/l = 0.4$  and values of the laser intensity  $V_0 = 0, 50$ , and  $100$ . Solution of  $\psi_1(\xi)$  taken from Ref. 24.

The choice of a test function that takes into account the variation shown in the figure will be treated in a future publication.

Also, the presence of two-species introduces an effective interaction of the unlike particle, which is described in our model by the coefficient  $\Lambda_3$ . The effect of the  $\Lambda_3 |\psi_j|^2 \psi_i$  term on the condensates is to attract ( $\Lambda_3 < 0$ ) or to repel ( $\Lambda_3 > 0$ ) the cloud probability densities  $|\psi_i(\xi)|^2$ . Thus, in the case we are dealing with a strong repulsive interaction, the maximum of the density probability lies at  $\xi \neq 0$ . Notice that the nature of our trial functions does not take into account the present peculiarity of two-species BEC. In Sec. V below we present a brief discussion of this effect.

### IV. PERTURBATION THEORY

Following the result of Eq. (20), we can write the system of coupled integral equations

$$\Psi(\xi) = \int_{-\infty}^{\infty} \mathbf{G}(\xi, \xi') [\mu - \mathcal{L}_I] \Psi(\xi') d\xi', \quad (31)$$

where the kernel

$$\mathbf{G}(\xi, \xi') = \begin{pmatrix} G_1(\xi, \xi') & 0 \\ 0 & G_2(\xi, \xi') \end{pmatrix}, \quad (32)$$

is the solution of the differential equations  $\mathcal{L}_0 \mathbf{G}(\xi, \xi') = I \delta(\xi - \xi')$  and  $I$  the identity matrix. In the spectral representation we have the Green function<sup>30</sup>

$$G_i(\xi, \xi') = \sum_{n=0}^{\infty} \frac{\varphi_n(\xi/l_i) \varphi_n(\xi'/l_i)}{(n+1/2)}, \quad i = 1, 2. \quad (33)$$

with  $l_i = \sqrt{a_i}$  and  $\varphi_n(z)$  is the harmonic oscillator wave-function.<sup>31</sup> Thus, inserting  $\mathbf{G}(\xi, \xi')$  in (31) we get

$$\Psi(\xi) = \begin{bmatrix} \psi_1(\xi) \\ \psi_2(\xi) \end{bmatrix} = \sum_{n=0}^{\infty} \begin{bmatrix} \sqrt{N_1} C_n \varphi_n(\xi/l_1) \\ \sqrt{N_2} D_n \varphi_n(\xi/l_2) \end{bmatrix}, \quad (34)$$

where the vectors  $\mathbf{C} = (C_1, C_2, \dots)$  and  $\mathbf{D} = (D_1, D_2, \dots)$  are given by

$$C_n[D_n] = \frac{1}{(n + \frac{1}{2})} \int_{-\infty}^{\infty} \left[ \left( \mu_{1[2]} - \lambda_{1[2]} |\psi_{1[2]}(\xi')|^2 + V_0 \cos^2(\alpha \xi') \right) + \lambda_3 |\psi_{2[1]}(\xi')|^2 \right] \varphi_n(\xi'/l_{1[2]}) \psi_{1[2]}(\xi') d\xi', \quad (35)$$

To satisfy Eqs. (34) and (35), the vector coefficients  $\mathbf{C}$  and  $\mathbf{D}$  must fulfill the non-linear system of equations

$$0 = \left[ \Delta^{(1)}(\mu_1) + \Lambda_1 \mathbf{C} \cdot \mathbf{T} \cdot \mathbf{C} + \Lambda_{12} \mathbf{D} \cdot \mathbf{S}(l_r) \cdot \mathbf{D} - V_0 \mathbf{P}(\alpha \sqrt{a_1}) \right] \mathbf{C}, \quad (36)$$

$$0 = \left[ \Delta^{(2)}(\mu_2) + \Lambda_2 \mathbf{D} \cdot \mathbf{T} \cdot \mathbf{D} + \Lambda_{21} \mathbf{C} \cdot \mathbf{S}\left(\frac{1}{l_r}\right) \cdot \mathbf{C} - V_0 \mathbf{P}(\alpha \sqrt{a_2}) \right] \mathbf{D}, \quad (37)$$

where  $l_r = \sqrt{a_1/a_2}$ ,  $\Delta_{nm}^{(i)} = (n + 1/2 - \mu_i) \delta_{nm}$ ,  $\mathbf{T}$  and  $\mathbf{P}(\alpha)$  are matrices given elsewhere<sup>24</sup> and  $\mathbf{S}(z)$  is defined in the Appendix A.

The above system is an infinite generalized eigenvalue problem for  $\mu_i$  ( $i = 1, 2$ ) and the vector coefficients  $\mathbf{C}$  and  $\mathbf{D}$ . An efficient algorithm for solving Eqs. (36)-(37) is presented in Ref.23. Nevertheless, it is very useful to carry with explicit expressions for  $\mu_i$  and  $\psi_i$  in terms of the leading parameters  $\Lambda$  and  $V_0$ . Assuming that the contribution of the non-linear terms and the optical potential appearing in the system (36)-(37) are small enough in comparison with that of the harmonic potentials, allows that the vector solutions  $\mu$ ,  $\mathbf{C}$  and  $\mathbf{D}$  can be sought as Taylor polynomials of the parameters  $\Lambda$  and  $V_0$ . Up to second order terms, and solving simultaneously the system (36)-(37), it is possible to show that the chemical

potentials is given by

$$\begin{aligned} \mu_{per,1} = & \frac{1}{2} + \frac{\Lambda_1}{\sqrt{2\pi}} + \frac{\Lambda_{12}}{\sqrt{\pi(1+l_r^2)}} - \frac{V_0}{2} [1 + \exp(-\alpha^2 a_1)] \\ & - 0.033106 \Lambda_1^2 + \frac{\sqrt{2} \Lambda_{12}}{\pi \sqrt{1+l_r^2}} \left[ 2\Lambda_1 f(l_r) + \Lambda_2 f\left(\frac{1}{l_r}\right) \right] \\ & + \frac{\Lambda_{12}}{\pi(1+l_r^2)} \left[ \Lambda_{12} g(l_r) + 2l_r \Lambda_{21} g\left(\frac{1}{l_r}\right) \right] + \\ & \frac{\exp(-\alpha^2 a_1) V_0}{\sqrt{2\pi}} \left[ \frac{\Lambda_{12}}{\sqrt{2(1+l_r^2)}} h\left(\frac{l_r^2 \alpha^2 a_1}{1+l_r^2}\right) + \right. \\ & \left. \Lambda_1 h\left(\frac{\alpha^2 a_1}{2}\right) \right] + \frac{\exp(-\alpha^2 a_2) V_0 \Lambda_{12}}{\sqrt{2\pi(1+l_r^2)}} h\left(\frac{\alpha^2 a_2}{1+l_r^2}\right) \\ & - \frac{\exp(-2\alpha^2 a_1) V_0^2}{4} ch(2\alpha^2 a_1). \quad (38) \end{aligned}$$

Functions  $f(z)$ ,  $g(z)$  and  $h(z)$  and  $ch(z)$  are defined in Appendix B.

Finally, the dimensionless order parameter,  $\psi_1$ , considering corrections up to the first order in  $\Lambda_1$ ,  $\Lambda_{12}$ , and  $V_0$ , can be expressed as

$$\begin{aligned} \psi_{per,1} = & \varphi_0(\xi) + \sum_{m=1}^{\infty} \left\{ \frac{(-1)^{m+1} \sqrt{(2m)!}}{\sqrt{\pi} 2^m (m!) 2m} \left[ \frac{\Lambda_1}{2^m \sqrt{2}} \right. \right. \\ & \left. \left. + \frac{\Lambda_{12}}{\sqrt{1+l_r^2}} \left( \frac{l_r^2}{1+l_r^2} \right)^m \right] + V_0 \frac{(-1)^m 2^{m-1}}{\sqrt{(2m)!}} \right. \\ & \left. \times (\alpha^2 a_1)^m \exp(-\alpha^2 a_1) \right\} \varphi_{2m}(\xi). \quad (39) \end{aligned}$$

The series, appearing in Eq. (39), can be summed obtaining the compact solution

$$\begin{aligned} \psi_{per,1} = & \varphi_0(\xi) + \Lambda_1 \mathcal{G}(\xi; \sqrt{2}) + V_0 \mathcal{F}(\xi, \alpha) \\ & + \Lambda_{12} \mathcal{G}(\xi; \sqrt{1+l_r^2}), \quad (40) \end{aligned}$$

where  $\mathcal{F}(x; \gamma)$  is reported in Ref.24 and  $\mathcal{G}(x; z)$  is defined in the Appendix B. For the chemical potential,  $\mu_{per,2}$ , and the order parameter for the second species,  $\psi_{per,2}$ , we obtain similar expressions by just changing  $1 \leftrightarrow 2$  and  $l_r \leftrightarrow 1/l_r$  in Eqs. (38) - (40).

## V. DISCUSSION OF THE RESULTS AND CONCLUSIONS.

In the following we present our results and discuss the reliability of the two implemented methods of solution. It will be useful to compare the obtained analytical expressions with direct numerical calculations. This comparison allows to find ranges of values of the parameters  $\Lambda_1$ ,  $\Lambda_2$ ,  $\Lambda_{12}$ ,  $\Lambda_{21}$  and  $V_0$  where the variational approach and perturbation method can be implemented for the description and predictions of the properties of the cigar-shape 1D two-species Bose-Einstein condensates. For the numerical evaluation of the system (20) we choose a finite difference method described in Ref.24.

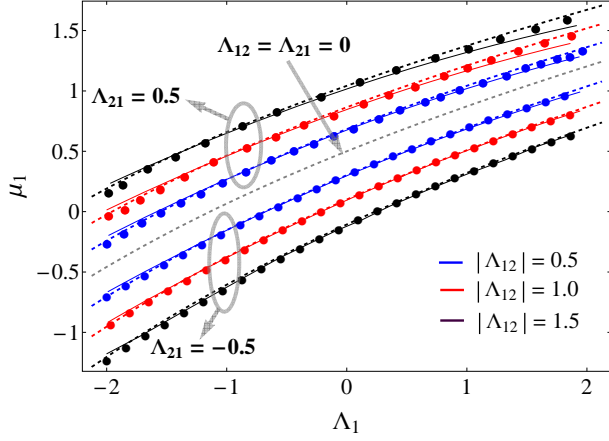


FIG. 2: (Color online) Dependence of the reduced chemical potential  $\mu_{per,1} = \nu_1/\hbar\omega$  on the dimensionless self-interaction parameter  $\Lambda_1$  for the inter-particle term  $\Lambda_{12} = \pm 0.5, \pm 1.0, \pm 1.5$  and  $\Lambda_{21} = \pm 0.5$ . Values of  $V_0 = 0$ ,  $l_r = 1$  and  $\Lambda_2 = 1$  are fixed. Dashed and solid lines represent the analytical results from Eqs. (27) and (38), respectively. Symbols correspond to the numerical solution of Eq. (6). For sake of comparison, the limit of one component ( $\Lambda_3 = 0$ ) using Eq. (27) is shown.

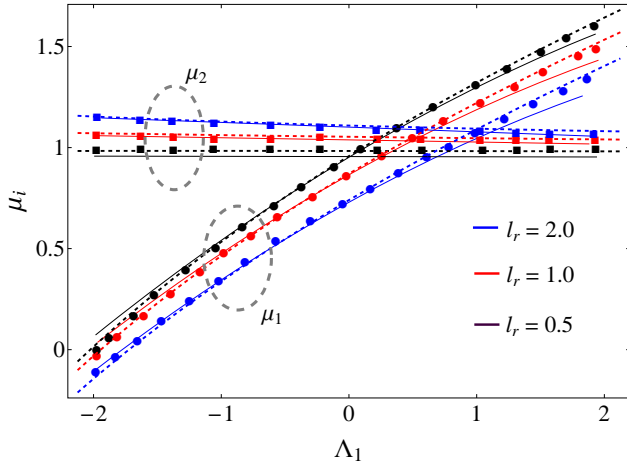


FIG. 3: (Color online) Dimensionless chemical potentials  $\mu_1$  and  $\mu_2$  as a function of  $\Lambda_1$  for several species ( $l_r = 0.5, 1.0$  and  $2.0$ ). The same nomenclature as in Fig. (2) are employed. In the calculation we sorted  $V_0 = 0$ ,  $\Lambda_2 = 1$ ,  $\Lambda_{12} = 1$  and  $\Lambda_{21} = 0.5$ .

### A. Chemical potentials

First, we analyze the case when the intensity of optical lattice is turned off,  $V_0 = 0$ . Figure (2) shows the reduced chemical potential  $\mu_1$  as a function of the dimensionless non-linear term  $\Lambda_1$  for the following values of the inter-species  $\Lambda_{12} = \pm 0.5, \pm 1$ , and  $\pm 1.5$ . In the calculation we have fixed  $\Lambda_2 = 1$ ,  $\Lambda_{21} = \pm 0.5$ , and  $l_r = 1$ . Variational approach calculations given by Eqs. (27) and (28) are in-

dicated by dashed lines, while the perturbation approach, using Eq. (38), is symbolized by solid lines. Symbols represent the results obtained by direct numerical evaluation of Eq. (6). Taking as reference the particular limit of one component, where  $\Lambda_3 = 0$ , as it is shown in Fig. 2, we observe that the influence of the inter-species interaction on the chemical potential is to increase  $\mu_1$  as the term  $\Lambda_{12} > 0$  increases, while the opposite result is achieved, i.e.,  $\mu_1$  decreases if  $\Lambda_{12} < 0$  decreases.

The small difference seen in the figure between the perturbation theory with respect to the variational and numerical solutions for  $\Lambda_1 > 0$  lies in the range of validity of Eq. (38). In Ref.25 it is shown that the perturbation theory for one component reproduces quite well the chemical potential if  $|\Lambda_1| \lesssim 2$ . In the present case, the inter-species interaction plays the role as an effective non linear term given by  $\Lambda_1 |\psi_1|^2 + \Lambda_{12} |\psi_2|^2$ . Hence, the range of validity of Eq. (38) as function of  $\Lambda_1 > 0$  is reduced if  $\Lambda_{12} > 0$ . The opposite we can argue if  $\Lambda_{12} < 0$ , i.e., the function  $\mu_{per,1}(\Lambda_1)$  given by (38) match the variational and numerical calculations in a large range of values of  $\Lambda_1 > 0$ . Similar arguments can be performed for the various combination of values of the parameters considered in Fig. 2.

In Fig. 3 we checked the influence of several species,  $l_r = 0.5, 1$ , and  $2$ , on  $\mu_1$  and  $\mu_2$  as function of  $\Lambda_1$  without optical lattice,  $\Lambda_2 = 1$ ,  $\Lambda_{21} = 0.5$ , and  $\Lambda_{12} = 1$ . As might be expected, the chemical potential  $\mu_2$  is almost constant as a function of the self-interaction term of the first species  $\Lambda_1$ . We note that for  $l_r > 1$  the value of the chemical potential  $\mu_1$  ( $\mu_2$ ) is reduced (increased), while the opposite it is obtained if  $l_r < 1$ . This result is explained by the fact that the effective inter-species  $\lambda_3 |\psi_i|^2$  depends on the mass ratio  $l_r$  (see Eqs. (6), (27), (28) and (38)).

It can be seen that the variational approach fits very well the numerical calculations, but the perturbation theory presents some differences as  $\Lambda_1 > 0$  ( $\Lambda_1 < 0$ ) increases (decreases). The same argument, as it is given in the analysis of Fig. 2, we can argue for the dependence of  $\mu_{per,i}$  on  $\Lambda_1$  and  $l_r$ . Nevertheless, this analysis has to be taken with caution. The presence of the functions  $f(z)$  and  $g(z)$  in Eq. (38) establishes different ranges of validity for  $\mu_i(\Lambda_1)$  as a function of  $l_r$ . Notice, that  $f(z) < 0$  for  $z > 0$ , while  $g(z) < 0$  ( $g(z) > 0$ ) for  $z > 1$  ( $z < 1$ ) (see Appendix B).

### B. Influence of the optical lattice

In Fig. 4 it is shown the behavior of the chemical potential as function of  $\Lambda_1$  for several values of the laser intensity  $V_0$ , the reduced wavelength  $\alpha$  and the  $\Lambda_{12}$  parameter. Solid lines represent the calculation following Eq. (38), dashed lines the variational approach as given by Eq. (27) with  $\Lambda_{12} = 0$ . Symbols correspond to the numerical solution of Eq. (6) for  $\Lambda_{12} = 0$ . From Fig. 4 it can be seen that Eq. (27) does not match with the per-

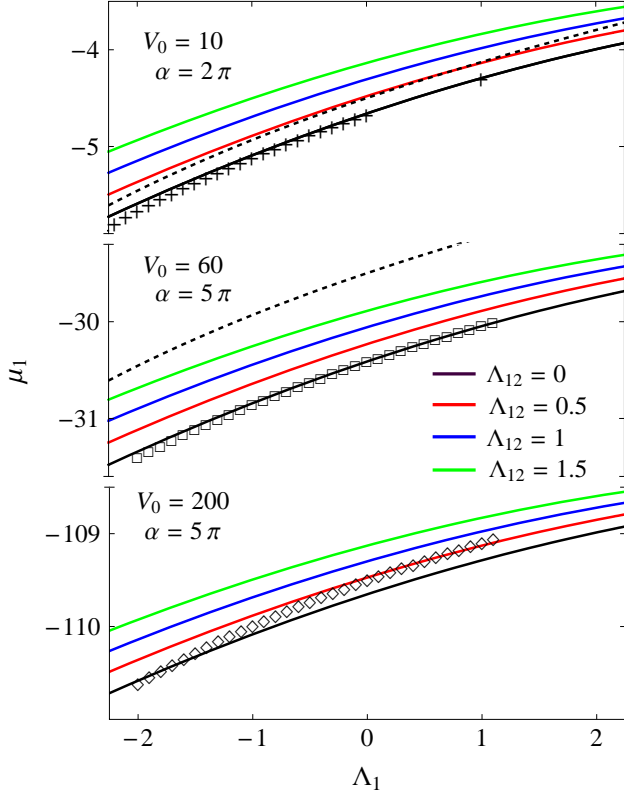


FIG. 4: (Color online) The same as Fig. 2 for several values of the reduced optical lattice intensity species ( $V_0 = 10, \alpha = 2\pi$  and  $V_0 = 60, 200$  with  $\alpha = 5\pi$ ). The influence of the interspecies interaction is represented by solid lines. Symbols are the numerical solution of the Eq. (6) and dashed lines the variation calculation using Eq. (27).  $\Lambda_2 = 1$  and  $\Lambda_{21} = 0.5$ .

turbation calculations neither numerical solutions. As  $V_0$  increases, the variational approach becomes worse, reflecting the choice of the trial functions (24) we have employed to calculate the energy. In connection with the perturbation theory, the agreement is satisfactory for any  $V_0$  less than 200, where a small deviation from the exact numerical results is achieved. As it is expected, the influence of the unlike interspecies interaction is to increase the chemical potential (the opposite is obtained if  $\Lambda_{12} < 0$ , not shown in the figure).

### C. Miscibility of the two species

A central issue for a description of the properties of multi species is the evaluation of the order parameter as a function of particle-particle and interspecies interaction. The control of the unlike particle interaction by Feshbach resonance<sup>4</sup> allows to tune the miscibility or not of these structures<sup>8</sup> and the challenge to create ultracold polar molecules.

Figure 5 displays the spatial distribution density

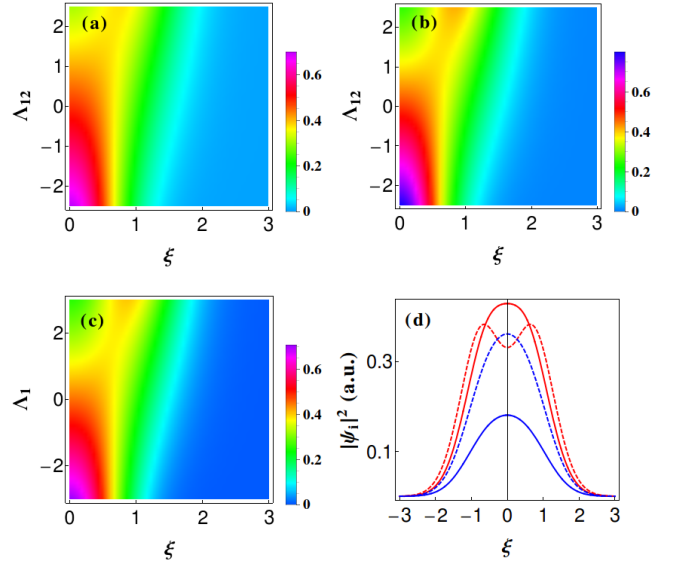


FIG. 5: (Color online) Density profile of the species BEC for  $V_0 = 0$ . Panel (a): As a function of  $\Lambda_{12}$  for  $\Lambda_1 = 1$  and  $l_r = 1$ . Panel (b): The same as panel (a) for  $l_r = 1.5$ . Panel (c): Varying  $\Lambda_1$  for  $\Lambda_{12} = 1$ , and  $l_r = 1.5$ . Panel (d): Functions  $|\psi_i(\xi)|^2$ ,  $i=1(2)$  red (blue) for  $\Lambda_{12} = 0.5$ ,  $N_2/N_1=0.8$  (solid line) and  $\Lambda_{12} = 0.8$ ,  $N_2/N_1=0.8$  (dashed lines). Here  $\Lambda_1 = 1$  and  $l_r = 1.5$ .

$|\psi_{per,1}(\xi)|^2$  as function of the dimensionless parameters  $\Lambda_{12}$  (panels (a) and (b)) and  $\Lambda_1$  (panel (c)). From Figs. 5(a) and (b) we observe the influence of one species over another. The condensate is more delocalized as the inter-species parameter  $\Lambda_{12}$  increases. Also, as the mass of the second species increases, the probability density  $|\psi_{per,1}(\xi)|^2$  spreads on the space and the maximum of the wavefunction decreases. The opposite is observed for the attractive interaction when  $\Lambda_{12} < 0$ , i.e., the density profile becomes more confined at  $\xi \approx 0$  as  $\Lambda_{12}$  decreases. Moreover, a stronger localization occurs as the parameter  $l_r$  increases. In other words, the system with large mass difference presents a more effective attraction between both components, which means that it favors the miscibility among both species if  $\Lambda_{12} < 0$ . A comparison between attractive and repulsive dimensionless non-linear parameter  $\Lambda_1$  is sorted in panel (c) of the figure. As  $\Lambda_1$  increases from 0 to 3, the density is spread in space. Also, for  $\Lambda_1$  large enough, the maximum of  $|\psi_{per,1}(\xi)|^2$  is displaced by the particle-particle repulsive interaction. In the case of attractive interaction,  $\Lambda_1 < 0$ , the maximum of the order parameter  $\psi_{per,1}(\xi)$  lies at the origin. For sake of clarity, in panel (d) we show the influence of the interaction  $\Lambda_{12}$  on the density profile  $|\psi_{per,i}(\xi)|^2$  ( $i=1,2$ ). Notice that the ground state is modulated by the repulsive interaction induced by the species 2 and the maximum of density probability is shifted to  $\xi \neq 0$  as  $\Lambda_{12}$  increases. From the physical point of view this results are clear, the species 2 is expelled off the origin



by the first condensate. The mutual repulsion between the two-species affect the spatial localization of density profile. As we stated above, this effect is driven not only by the values of  $\Lambda_{12}$ , but also by the ratio of the masses involved in the two condensates (see Eq. (40)).

The density distributions results of Fig. 5 indicate in a general way the degree of the immiscibility or phase separation of binary condensate due to the interspecies repulsion. In our case the structure is symmetric and it is related with the ratio of number of particles  $N_2/N_1$ . These results are in complete concordance with recent experimental reported observations for the  $^{87}\text{Rb}$  -  $^{133}\text{Cs}$  binary condensates.<sup>5</sup> The trial wavefunctions (24) cannot take into account these behaviors over the spatial distribution as a function of  $\Lambda_{12}$ , since they are *a priori* located at the origin.

In conclusion, we have derived simple explicit expressions for the chemical potentials and order parameters in the case of two species of non-homogeneous BEC, where the system is loaded in a harmonic trap potential. We generalize the variational method for the case of two coupled GP equations, showing that the obtained closed analytical expressions for  $\mu_i$  ( $i = 1, 2$ ) represent very good solutions for any values of the vector  $\mathbf{\Lambda}$  if  $V_0 = 0$ . Also, employing the perturbation theory we are able to get analytical solutions for  $\mu_i$  and the order parameter components  $\psi_i$  as functions of the dimensionless vector  $\mathbf{\Lambda}$ . By comparison with the numerical solutions we found the range of validity of the Eq. (38). By the calculations we show the strong dependence of  $\mu_i$  and  $\psi_i$  on the strengths  $\Lambda_1$ ,  $\Lambda_2$ ,  $\Lambda_{12}$ ,  $\Lambda_{21}$  and  $V_0$ . This study gives a very useful result establishing the universal range where each solution can be easily implemented. In particular, the dependence of the order parameter  $\psi_i$  on  $\Lambda_i$  and  $\Lambda_{ij}$  ( $i \neq j$ ) allows to study the immiscibility of two given species. We should note that the variational model here developed can be extended to a cubic-quintic model<sup>20</sup> and allows to explore the influence of quintic nonlinear terms on the ideal 1D two coupled pure cigar-like shape system.

### Acknowledgements

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### Appendix A: Matrix elements

The fourth dimensional matrix  $\mathbf{S}(l_r)$  is defined as

$$S_{mn;pl}(l_r) = \frac{1}{\pi \sqrt{2^{n+m+l+p} n! m! l! p!}} \times \int_{-\infty}^{\infty} [\exp[-(1+l_r^2)z^2] H_n(z), H_m(z) H_l(l_r z) H_p(l_r z)] dz, \quad (\text{A1})$$

with  $H_n(z)$  the Hermitian polynomials<sup>32</sup>. The matrix elements  $S_{mn;pl}(l_r)$  have the followings properties:

- i)  $l_r S_{mn;pl}(l_r) = S_{pl;mn}(1/l_r)$ ;
- ii)  $S_{2m0;00}(l_r)$ ,  $S_{k0;0m}(l_r)$  and  $S_{km;00}(l_r)$  are equal to<sup>33</sup>

$$S_{2m0;00}(l_r) = \frac{(-1)^m \sqrt{(2m)!}}{\sqrt{\pi(1+l_r^2)} 2^m m!} \frac{l_r^{2m}}{(1+l_r^2)^m}, \quad (\text{A2})$$

$$S_{k0;0m}(l_r) = \frac{(-1)^{\frac{3m+k}{2}} (k+m)!}{\sqrt{\pi} \sqrt{k!m!} 2^{\frac{m+k}{2}} \left(\frac{k+m}{2}\right)!} \frac{l_r^k}{(1+l_r^2)^{\frac{m+k+1}{2}}},$$

$$S_{km;00}(l_r) = \frac{(-1)^{\frac{k+m}{2}} 2^{\frac{m+k}{2}} \Gamma\left(\frac{k+m+1}{2}\right) l_r^{k+m}}{\pi \sqrt{k!m!} (1+l_r^2)^{\frac{m+k+1}{2}}} F\left(-k-m, \frac{1-k-m}{2}; \frac{1+l_r^2}{2l_r^2}\right), \quad (\text{A3})$$

with  $\Gamma(z)$  the Gamma function<sup>32</sup> and  $F(\alpha, \beta; z)$  the confluent hypergeometric function.<sup>33</sup>

Using the above relations it is possible to get Eqs. (38)-(40).

### Appendix B: Functions

The functions introduced in Eq. (38) are defines as:

$$f(z) = \ln \left[ \frac{1}{2} + \frac{1}{2} \sqrt{\frac{2+z^2}{2(1+z^2)}} \right], \quad (\text{B1})$$

$$g(z) = \ln \left[ \frac{1}{2} + \frac{1}{2} \sqrt{\frac{1+2z^2}{(1+z^2)^2}} \right] \quad (\text{B2})$$

$$h(z) = Ei(z) - \mathcal{C} - \ln z; \quad ch(z) = Chi(z) - \mathcal{C} - \ln z, \quad (\text{B3})$$

where  $Ei(z) = \int_{-\infty}^z \frac{\exp(x)}{x} dx$  is the exponential integral,  $Chi(z)$  the cosine hyperbolic integral, and  $\mathcal{C}$  the Euler's constant.

In Eq. (40) the  $\mathcal{G}(\xi; z)$  is given by

$$\mathcal{G}(\xi; z) = \frac{\exp(-\xi^2/2)}{z \sqrt{\pi} \sqrt{\pi^{1/2}}} \int_1^{1/z} \frac{\exp\left[-\frac{\xi^2}{y^2} (1-y^2)\right] - 1}{1-y^2} dy. \quad (\text{B4})$$

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